Indoline, 1-(2-pyridylmethyl)-

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 128 °C

Global applicability domain: Inside

Local applicability domain index: 6.48e-01

Confidence level: 4.12e-01

Nearest Neighbors from the Training Set

Image not found
Pyrimidine, 4-phenyl-
Measured: 56.0
Predicted: 72.3

Image not found
Imipramine
Measured: 175
Predicted: 145

Image not found
Imipramine hydrochloride
Measured: 174
Predicted: 145

Image not found
Clomipramine
Measured: 190
Predicted: 163

Image not found
Trimipramine
Measured: 45.0
Predicted: 119